1/4

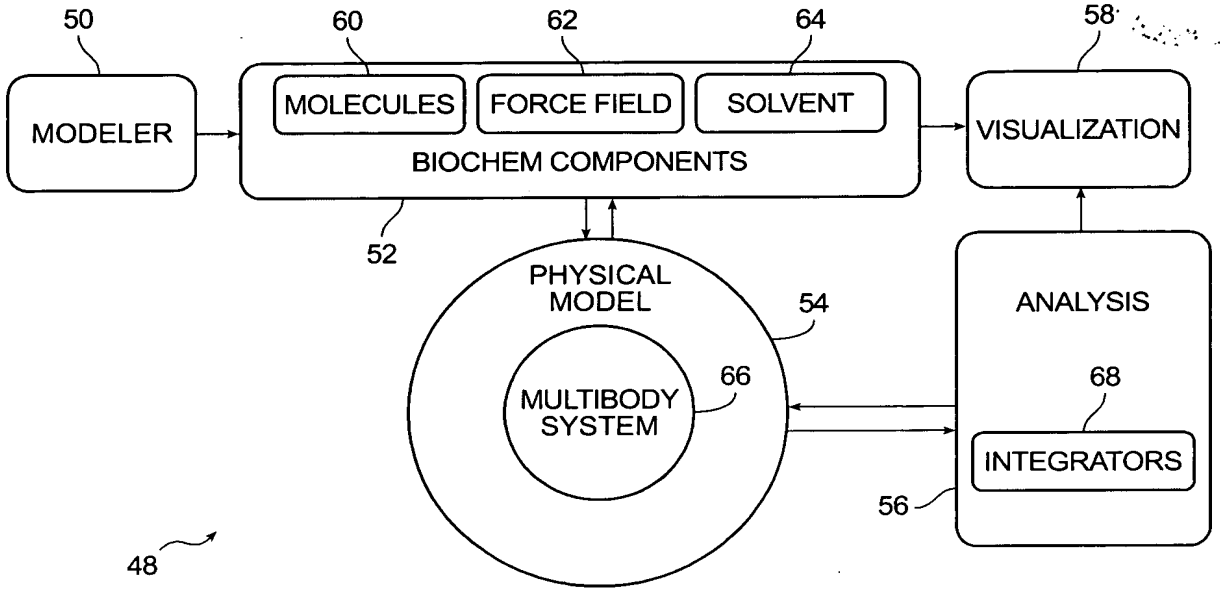
50
60
62
64
58
MODELER
MOLECULES
FORCE FIELD
SOLVENT
BIOCHEM COMPONENTS
VISUALIZATION
52
PHYSICAL MODEL
54
ANALYSIS
MULTIBODY SYSTEM
66
68
INTEGRATORS
56
48

FIG. 1

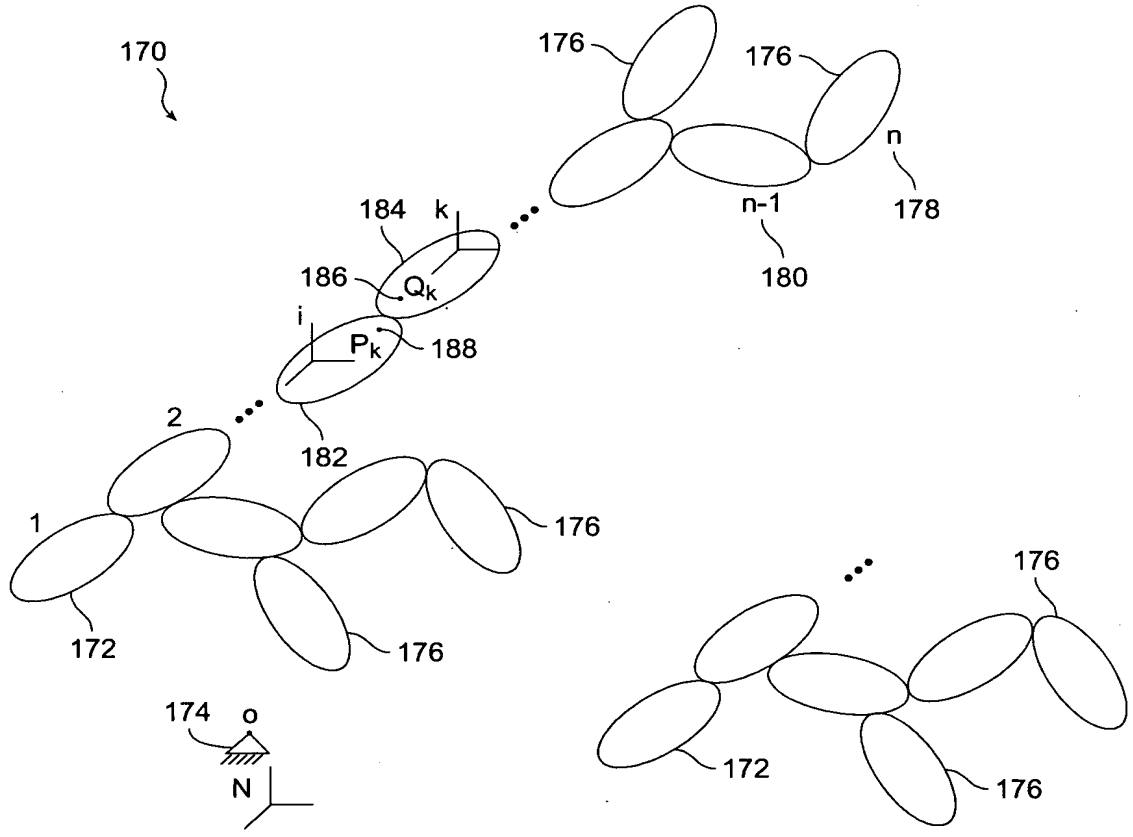
170
176
176
n
n-1
178
180
184
k
186
Q_k
i
P_k
188
2
182
1
176
172
176
174
o
N
176
172
176

FIG. 2

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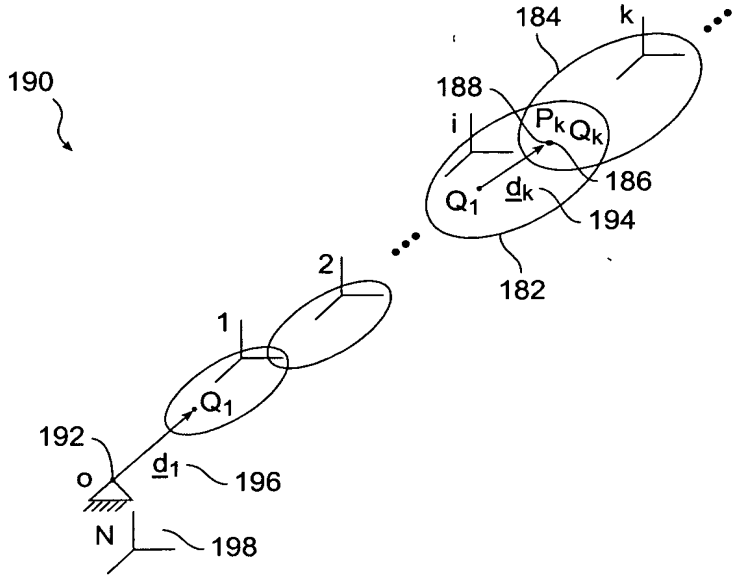

FIG. 3

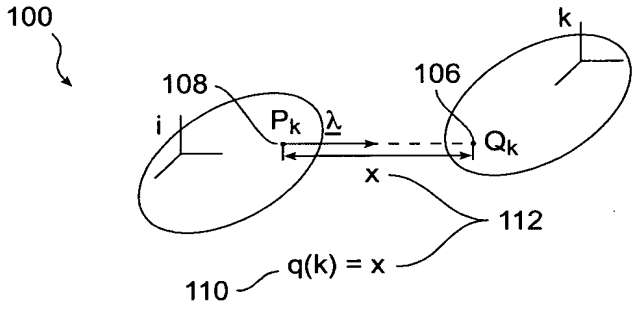

FIG. 4A

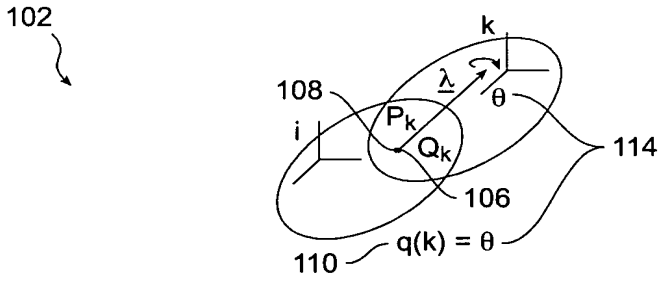

FIG. 4B

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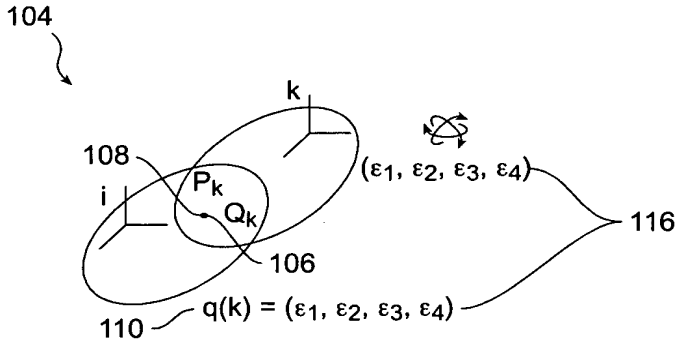

FIG. 4C

RESIDUAL FORM METHOD TO COMPUTE ρ_q AND ρ_u	DIRECT FORM METHOD TO COMPUTE $\dot{q}$ AND $\dot{u}$
1. COMPUTE THE FIRST KINEMATICS CALC. AND THE FIRST KINEMATIC RESIDUAL $\rho_q(k)$ 2. GENERATE $\hat{T}(k)$, THE SPACIAL LOAD BALANCE FOR EACH BODY 3. COMPUTE DYNAMIC RESIDUAL $\rho_u(k)$	1. COMPUTE $\dot{q}$ USING JOINT SPECIFIC ROUTINES 2. PERFORM FIRST KINEMATICS CALC. WITH $\dot{u} = 0$ 3. GENERATE RESIDUALS ρ_u AND NEGATE $\rho_u = -\rho_u$ 4. PERFORM SECOND KINEMATICS CALC. 5. COMPUTE $\dot{u}$ USING FORWARD DYNAMICS

COMPARISON OF METHODS

FIG. 5

MOLECULE	NO. RESIDUES IN POLYPEPTIDE	NO. ATOMS	DIRECT FORM APPROXIMATE OPERATION COUNT	RESIDUAL FORM APPROXIMATE OPERATION COUNT	FACTOR OF SPEED UP
ALANINE DIPEPTIDE	2	23	4,991	683	7.31
20-MER POLYALANINE	20	257	42,340	5,894	7.24
100-MER POLYALANINE	100	1297	207,018	28,973	7.15

COMPUTATION COMPARISON

FIG. 6